Short-range correlations and spin-mode velocities in ultrathin one-dimensional conductors

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In ultrathin wires positioned on high-κ dielectric substrates or nearby metallic gates, electrons can form strongly correlated one-dimensional fluids already at rather high electron densities. The density-density correlation function, charge compressibility, spin susceptibility, and electron specific heat of such fluids are calculated analytically. The results are relevant for transport and thermodynamics of carbon nanotube field-effect transistors and semiconductor quantum wires.

There is a long-standing theoretical prediction that one-dimensional (1D) electrons do not obey the conventional Fermi-liquid theory but instead form a Luttinger liquid (LL)[1] whose fundamental degrees of freedom are bosonic modes that separately carry electrons' charge and spin. Experimental verification of the LL theory has proved to be a challenge. There is, however, evidence for a LL-specific suppression of tunneling into carbon nanotubes (CN)[2] and a spin-charge separation in quasi-1D organics.[3] Vexing questions remain: (1) Is there a way to demonstrate a truly dramatic departure from the Fermi-liquid in real 1D systems? (Aside from the special case of quantum Hall edge states.[4]) And if so: (2) What theory should one use to describe such a regime in the presence of long-range Coulomb interactions? Finally, (3) What phenomena can one expect from this deeply non-Fermi-liquid state? Below we propose that the desired strong coupling regime can be realized if an *ultrathin* wire, e.g., a CN is (i) placed on a high-κ dielectric substrate or (ii) brought close to a metallic gate. In contrast, the traditional prescription for obtaining a strongly correlated regime is to lower the electron density n thereby increasing the Coulomb coupling constant $r_s = 1/2na_B$, where $a_B = \hbar^2\kappa/m_*e^2$ is the effective Bohr radius. Unfortunately, this route quickly runs into the problem of localization by disorder, e.g., random charges on the substrate. The advantage of our proposal is that the Coulomb potential of these charges would be strongly screened, whereas interactions among electrons would be affected much less, as shown below.

We begin with the dielectric substrate case. We call a wire of radius R *ultrathin* if $R \ll a_B$. Experimentally, enormous $a_B/R \sim 10^4$ ratios are achievable in devices that use zigzag CNs[6] placed on the $SrTiO_3$ substrate[5] ($R \sim 1\,\mathrm{nm}$, $\hbar^2/m_*e^2 \sim 50\,\mathrm{nm}$, $\kappa \sim 200$). We show that in such an ultrathin wire Coulomb correlations are enhanced by a large parameter $\mathcal{L} = \ln(a_B/R)$ and a correlated regime — Coulomb Tonks Gas (CTG) — appears in a window $\mathcal{L}^{-1} \ll r_s \ll 1$ of *low* r_s. The CTG can be defined as the state where on all but exponentially large lengthscales, $x < x_* = a_B \exp(\pi^2/2r_s)$, electrons behave as a gas of impenetrable but otherwise free fermions. At such x the LL theory, being an asymptotic *long-wavelength* theory, has no predictive power, and the alternative method presented below is needed; $x_* \sim 1\,\mu\,\mathrm{m}$ should be achievable in current CN devices.[5] The CTG owes its name to a certain similarity it enjoys with the Tonks-Girardeau gas of 1D cold atoms.[7]

We find that to the leading order in $1/\mathcal{L} \ll 1$, the short-range *density* correlations in the CTG are identical to those of a one-component free Fermi gas. The *spin* correlations are the same as in the 1D antiferromagnet. We show that the CTG possesses a number of properties akin to the $r_s \gg 1$ 1D Wigner crystal,[8] including a negative compressibility, a high spin susceptibility and electron specific heat, and also anomalous finite-temperature transport[9] and tunneling[10] properties. Thus, although the 1D Fermi gas, the CTG, and the Wigner crystal are not different thermodynamical phases (they all are LLs), significant quantitative differences in short-range properties of the electron system in these three regimes cause sharp crossover changes in the observables, similar to the boson case.[7]

Let us proceed to the derivation of these results. The crucial insight comes from the two-body problem. Consider two electrons with a relative momentum $q \sim 1/a = 1/2r_sa_B$ interacting via a model potential $U(x) = e^2/\kappa(|x| + R)$. We face the following puzzle. If $r_s \ll 1$, we have the inequality $e^2/\kappa\hbar v \ll 1$, so that the kinetic energy greatly exceeds the characteristic Coulomb energy ($v = \hbar q/m_*$ is the relative velocity). Naively, one may expect that the Coulomb potential should be a small perturbation. But the reflection coefficient computed in the first Born approximation is equal to $i\ln(Rq)/a_Bq$, which is large in the range of r_s that corresponds to the CTG. To resolve this puzzle one has to separate the effects of the tails of the Coulomb potential (large-x) and of its sharp increase at the origin (small-x). Indeed, let us examine the Schrödinger equation for the wavefunction ϕ of the relative motion

$$-\phi''(\xi) + \frac{r}{|\xi| + \alpha}\phi - \frac{1}{4}\phi = 0, \qquad (1)$$

where $\xi = qx$ is the dimensionless separation, $r = 1/qa_B$, and $\alpha = Rq$. We focus on the case $r \sim r_s \ll 1$, $\alpha \ll 1$.

The general solution of Eq. (1) is given by

$$\phi(\xi) = A_sW_{ir,\frac{1}{2}}(i|\xi| + i\alpha) + B_sW_{-ir,\frac{1}{2}}(-i|\xi| - i\alpha), \quad (2)$$

where $s = \mathrm{sgn}(\xi)$ and $W_{\mu,\nu}(z)$ is the Whittaker function.[11] The constants A_s and B_s must be chosen to en-

sure the continuity of ϕ and ϕ' at $\xi = 0$. The Whittaker function has the asymptotic behavior[11]

$$W_{ir,1/2}(i\xi) \sim \exp[-i(\xi/2) + ir\ln(\xi) - \pi r], \quad \xi \gg r. \quad (3)$$

Due to the logarithm in Eq. (3), which results from the slowly decaying $1/|x|$-tail of the interaction potential, the scattered states are not exactly plane waves. Thus, if $t(q)$ denotes the transmission amplitude, its phase depends on the distance x from the origin to the points where the scattered states are measured, $t(q) \propto \exp[-ir\ln(xq)]$. However, in a wide range of x, from the classical turning point $x \sim r/q \sim a^2/a_B$ to an exponentially large distance $x \sim q^{-1}\exp(1/r) \sim a\exp(1/r_s)$, this dependence of $t(q)$ is very slow. The phase shift accumulated over this entire interval of x is small and can be ignored. This is consistent with Coulomb potential being a small perturbation at such x. Note that the point $x \sim 1/q$, which corresponds to the the characteristic interelectron distance a in the many-body problem, is safely within the indicated range of x. Therefore, for our purposes we can define the transmission coefficient by $t(q) \equiv B_+/A_-$ at $A_+ = 0$. With this definition, one can show that $t(q)$ is given by

$$t(q) = i\exp(-\pi r)[(d/d\alpha)W^2_{-ir,1/2}(-i\alpha)]^{-1}, \quad (4)$$

which entails (cf. Ref. 11)

$$t(q) = \frac{iq}{iq - c(q)}, \quad c = -\frac{2\ln(Rq)}{a_B}, \quad qa_B \gg 1. \quad (5)$$

Thus, there exists a window of momenta, $1/a_B \ll q \ll \mathcal{L}/a_B$, where the Coulomb barrier is effectively impenetrable (opaque),[12] $|t(q)| \ll 1$, due to the strong backscattering at an exponentially short approach distance, $x \sim q^{-1}\exp(-qa_B)$. We conclude that while the tails of the Coulomb potential act as a small perturbation at momenta $q \sim k_F \equiv \pi n$ and distances $x \sim a$, which are the most relevant for the many-body problem, the strong *short-range* repulsion yields the effective hard-core constraint for the charge dynamics. Therefore, in the first approximation the Coulomb potential is equivalent to a very thin and high barrier, i.e., to a δ-function of a large strength. Equation (5) supports this identification because up to $O(1/\mathcal{L})$-terms, $t(q)$ coincides with the transmission amplitude for the potential

$$U(x) = (\hbar^2/m_*)c(k_F)\delta(x). \quad (6)$$

Note that in the opposite limit $r \ll 1$ of a low-energy scattering the tails of the Coulomb potential cannot be ignored. The point of interest $x \sim q^{-1}$ resides deeply inside a classically forbidden region of the Coulomb barrier where the wavefunction ϕ depends exponentially on x. This regime will not be important in what follows, but for future reference we quote the counterpart of Eq. (5), $|t(q)| \simeq (\pi/\mathcal{L})\exp(-\pi/qa_B)$. Let us now apply the above ideas to the analysis of the many-body problem.

Consider the limiting case $R = +0$ first. We have $c = \infty$ and $t(q) = 0$ for all q; hence, the ground-state wavefunction Ψ has a node whenever coordinates x_j of any particles coincide, $1 \le j \le M$. Using an argument similar to Lieb-Mattis theorem,[13] one can show that Ψ has no other nodes. Thus, it must have the form

$$\Psi = \exp[W(x_1,\ldots,x_M)] \prod_{Qi>Qj} \sin\frac{\pi}{L}(x_{Qi} - x_{Qj}) \quad (7)$$

$$\times\ (-1)^Q\Phi(s_1,\ldots,s_M) \quad (8)$$

where $Q1$ through QM are the indices in the ordered list of the electron coordinates $0 < x_{Q1} < \ldots < x_{QM} < L$ (periodic boundary conditions are assumed), $(-1)^Q$ is the parity of the corresponding permutation, s_j is the spin of Qjth electron, and Φ is the spin part of the wavefunction. The factor $\exp(W)$ incorporates the effect of weak $1/x$-tails of the interaction. Apart from this, Ψ coincides with the ground-state of electrons with infinitely strong δ-function repulsion,[18] i.e., the gas of impenetrable but otherwise free fermions (GIF). Below we focus on correlation functions for which W is not needed directly.

Due to the strict impenetrability built into Ψ, particle exchanges are forbidden, and so neither the parity factor $(-1)^Q$ nor spin are dynamical degrees of freedom. (So, at $R = +0$ extra assumptions are needed to fix Φ). All correlation functions are slaved to those of the density operator $\rho(x)$, e.g., the two-point cluster function,

$$h(x) = a^2\langle\Psi|\rho(x)\rho(0)|\Psi\rangle - 1, \quad (9)$$

In the GIF ($W = 0$) $h(x)$ is the same[18] as in the spin-polarized Fermi gas with the Fermi momentum $k_F = \pi n$,

$$h(x) = -\sin^2(k_Fx)/(k_Fx)^2, \quad (10)$$

$$\tilde{h}(q) = -a + \theta(2k_F - q)q/(2k_Fn), \quad (11)$$

where $x, q^{-1} \ll L$, $\theta(z)$ is the step-function, and henceforth the tilde denotes the Fourier transform.

The tails of the Coulomb potential cause a correction $\delta h(x)$ to Eq. (10). From the analysis of the two-body problem, we expect that at not too small x, $\delta h(x)$ admits a diagrammatic expansion in r_s. Since the term $(-1)^Q\Phi$ does not affect the dynamics, this expansion has identically the same form as for one-component fermions, so that the standard calculation yields, in the leading order

$$\delta\tilde{h} \simeq -\frac{r_s}{\pi^2}\frac{q}{k_Fn}\ln\frac{2k_F}{q}, \quad q \ll 2k_F, \quad (12)$$

$$\sim \delta h(2k_F) + \frac{r_s|z|}{\pi^2 n}\ln^2|z|, \ z = \frac{2k_F - q}{2k_F} \to 0, \quad (13)$$

$$\simeq \frac{8}{\pi^2}\frac{r_s}{n}\frac{k_F^4}{q^4}, \quad q \gg 2k_F. \quad (14)$$

As one can see, $\delta h(x)$ is a small correction to $h(x)$ [Eq. (10)] up to an exponentially large distance $x_* \sim a\exp(\pi^2/2r_s)$. We show below that these first-order results for $\delta h(x)$ smoothly match at $x \sim x_*$ with the asymptotic long-distance behavior of $h(x)$ computed from the LL theory, which is supposed to resum the

perturbative series to all orders. We conclude that at $r_s a \ll x \ll x_*$ the first-order perturbation theory applies and that the charge correlations in the CTG are indeed no different from those of free spinless fermions.

This result suffies to demonstrate that the compressibility of the CTG is negative. We define the inverse compressibility by $\varkappa^{-1} = d^2\varepsilon/dn^2$, where $\varepsilon(n)$ is the energy density of the system. To make it finite the Hartree term (interaction with a neutralizing uniform backround) must be subtracted away. This is an important difference from the case of short-range interactions. To the leading order in r_s, ε is equal to the kinetic energy of the spin-polarized Fermi gas plus the potential energy evaluated using Eq. (11) for $\tilde{h}(q)$. This simple calculation gives

$$\varkappa^{-1} = -\frac{2e^2}{\kappa}\left[\mathcal{L} - \frac{\pi^2}{4r_s} + \ln\left(\frac{2r_s}{\pi}\right) - \gamma\right], \qquad (15)$$

which is indeed negative at $1/\mathcal{L} \ll r_s \ll 1$. Here γ is the Euler constant.[11] With our definition of $\varkappa$, its negative sign does not imply any instability of the CTG towards, e.g., phase separation. The phase separation would cost a large Hartree charging energy that would outweigh any gain due to negative $\varkappa^{-1}$ term.[14]

Let us briefly make a connection with the LL theory. The above result for $\varkappa$ enters the LL machinery through the charge stiffness parameter

$$K_\rho(q) = \sqrt{\frac{(\pi/4)\hbar v}{\tilde{U}(q) + \varkappa^{-1}}}, \quad v = \pi\frac{\hbar n}{m_*}. \qquad (16)$$

Unlike the "classical" definition,[1] in a Coulomb LL[8,16,17] K_ρ depends not only on $\varkappa$ but also on the interaction potential $\tilde{U}(q) \sim -2(e^2/\kappa)\ln Rq$. This is again because the total energy cost of the charge build-up is the sum of the negative $\varkappa$-term (correlation energy[15]) and the large postitive Hartree term (electrostatic energy). K_ρ shows up [through $v_c(q) = v_F/K_\rho(q)$] in the dispersion $\omega = v_c(q)q$ of charge mode. It also determines the low-q behavior of the density correlation function:

$$\tilde{h}(q) + a \sim -K_\rho(q)q/(k_F n), \quad q \to 0. \qquad (17)$$

We notice that Eqs. (12) and (17) match at $q \sim 1/x_*$ and take it as evidence that Eq. (17) applies at $q < 1/x_*$, while Eq. (12) is valid at $q > 1/x_*$. Thus, the first-order perturbation theory is sufficient for computing $h(x)$ at $x < x_*$. The LL theory can also be used to calculate the crossover from Eq. (13) to a different type of singularity in the immediate vicinity of $q = 2k_F$. If desired, one can use this to study in detail how the asymptotic $\exp[-\sqrt{r_s\ln(x/x_*)}]$ decay[8,16,17] of the "$2k_F$" ($2a$-periodic) oscillations of $h(x)$ is recovered at large x.

So far, we have discussed the case of an infinitely thin wire. If R is finite, Ψ has nodes only at the coincident positions of the same-spin particles. However, due to the opacity of the Coulomb barrier in the CTG, $h(x)$ is perturbed very slightly. A much more important difference is that particle exchanges become allowed and the spin acquires some dynamics. Thus, it becomes meaningful and interesting to determine Φ. Since particle exchanges are still highly suppressed, only those between nearest neighbors are relevant. In the CTG they are determined by the two-body transmission amplitude $t(q)$. Recall that the orbital part of the scattered wave depends on the total spin $\mathbf{S} = \mathbf{S}_1 + \mathbf{S}_2$ of the two colliding particles,

$$\phi = e^{i\xi/2} \pm e^{-i\xi/2} + [t(q) - 1](e^{i|\xi|/2} \pm e^{i|\xi|/2}), \qquad (18)$$

where the upper (lower) sign is for the singlet (triplet). To the order $O(t)$, exactly the same asymptotic scattered wave would result from the exchange coupling $U_{\text{eff}} = (\mathbf{S}_1\mathbf{S}_2 - 1/4)U_\sigma(x)$ if at all k such that $|t(k)| \ll 1$ we have $\tilde{U}_\sigma(k) = 2(\hbar^2/im_*)t(k)k + \text{const}$, as can be readily verified via Born approximation. Although the form of the short-range potential $U_\sigma(x)$ in the real space is not unique, this has no significance to the first order in the small parameter t. Therefore, the spin-spin interaction is captured by the Hamiltonian

$$H_\sigma = \frac{\hbar^2}{m_*}\int\frac{dk}{2\pi}\left(\mathbf{s}_k\mathbf{s}_{-k} - \frac{1}{4}\rho_k\rho_{-k}\right)\text{Im}\, t(k)k, \qquad (19)$$

where the integration is to be done up to the ultraviolet cutoff $k_{\max} \lesssim c(k_F)$ and $\mathbf{s}_k$, ρ_k are the harmonics of the spin and charge densities at wavevector k. The physical idea expressed by Eq. (19) is very similar to that behind the familiar antiferromagnetic coupling $(4t^2/U)(\mathbf{S}_i\mathbf{S}_{i+1} - n_i n_{i+1}/4)$ in a large-U 1D Hubbard model.[19]

Since the spins are slow degrees of freedom, we can average H_σ over the fast orbital motion to obtain the usual 1D $S = 1/2$ Heisenberg model

$$H_\sigma = J\sum\nolimits_j \mathbf{S}_j\mathbf{S}_{j+1}, \quad J = \frac{\hbar v}{2\pi^2}\int\tilde{h}(k)\text{Im}\, t(k)kdk. \qquad (20)$$

Therefore, the spin wavefunction Φ for the ground and excited states are given by the appropriate Bethe ansatze.[20] Substituting Eq. (5) into Eq. (20) and keeping only terms $O(1/\mathcal{L})$, we obtain

$$J = \frac{\pi^2}{3}\frac{\hbar^2}{m_*}\frac{n^3 a_B}{\mathcal{L} + \ln r_s}, \quad \frac{1}{\mathcal{L}} \ll r_s \ll 1. \qquad (21)$$

In the CTG, $J \ll E_F \equiv \hbar^2 k_F^2/8m_*$, as expected. The velocity of the spin excitations in 1D Heisenberg model is[20] $v_\sigma = (\pi/2)(Ja/\hbar)$ and the spin susceptibility per unit length is $\chi_\sigma = (g\mu_B/2)^2(2/\pi\hbar v_\sigma)$. This implies that χ_σ of the CTG exceeds that of the Fermi gas χ_σ^0 (where $v_\sigma = v/2$) by the large factor $\chi_\sigma/\chi_\sigma^0 = v/2v_\sigma \approx r_s\mathcal{L} \gg 1$.

The low-temperature electron specific heat of a CTG is determined by the velocities of the charge and the spin modes[18] and is dominated by the latter, $C_e = (\pi/3)(k_B T/\hbar v_\sigma) \sim (2/\pi^2)(\kappa/e^2)(r_s^2/\mathcal{L})k_B T$. This is large compared to C_e in the Fermi gas because of the smallness of v_σ. Obviously, v_σ is relevant for many observables. To verify that our strategy for finding v_σ is correct, we made sure that it reproduces the known exact

results[18,19] for the 1D Hubbard model and for electrons with the contact interaction (6),

$$v_\sigma \simeq (\pi^3/3)(\hbar n^2/m_* c), \quad n \ll c. \tag{22}$$

A gated wire.— Properties similar to those of the CTG may also be exhibited by a modestly thin 1D wire, $R \lesssim a_B$, if, instead of a high-κ dielectric, it is positioned a small distance D away from a metallic gate. In that case one can model the interaction potential by $U(x) = e^2/|x| - e^2/\sqrt{x^2+4D^2}$ at $|x| \gg R$. This model was studied recently by Häusler *et al.*[21] who surmised that $K_\rho \to 1/2$ and $v_\sigma \propto n^2/\ln(D/R)$ at low n. In the regime $a \gg D^2/a_B \gg a_B$ the validity of these statements can be examined in a controlled fashion. The interaction potential is short-range, $U(x) \propto x^{-3}$ at $x \sim a$, and opaque, so the system is in the GIF limit. After a straightforward calculation of $t(q)$ one finds that c in Eq. (5) has to be replaced by[22]

$$c = A\frac{a_B}{D^2}\exp\left\{\sqrt{\frac{\pi D}{2a_B}}\left[\frac{\Gamma(1/8)}{\Gamma(5/8)} + \frac{\Gamma(5/8)}{\Gamma(9/8)}\right]\right\}, \tag{23}$$

where coefficient $A \sim 1$ depends on the behavior of $U(x)$ at $x \sim R$, and $\Gamma(z)$ is Euler's gamma function.[11] Since the interaction potential is now short-range, subtraction of the Hartree term is no longer necessary. We redefine $\varkappa^{-1} + \tilde{U}(q=0) \to \varkappa^{-1}$ and obtain $\varkappa^{-1} = \pi^2 e^2 a_B n$. Equation (16) then implies that $K_\rho \simeq 1/2$; however, the spin velocity, which can be found by substituting Eq. (23) into Eq. (22), differs from the surmise of Ref. 21.

Experimental manifestations.— The predicted large difference of spin and charge mode velocities (v_c and v_σ) can be verified by momentum-resolved photoemission[3] or tunneling.[23] Since CN is currently the best candidate for realizing the Coulomb Tonks Gas regime, we have to mention here that the bands of a pristine CN have a two-fold valley degeneracy. This can be accommodated into the model via effective spin-1/2 operators $\mathbf{T}_i$. Each two-body term in Eq. (20) should then be replaced by $J(\mathbf{S}_i\mathbf{S}_{i+1} + 1/4)(2\mathbf{T}_i\mathbf{T}_{i+1} + 1/2)$. The resultant H_σ remains integrable[24] and one finds that now $v_\sigma = (\pi^3/6)(\hbar n^2/m_* c)$. Transport is another powerful probe of the CTG and Wigner crystal regimes. In the temperature window $J \ll k_B T \ll E_F$, with $J \sim 1\,\mathrm{K}$ (a crude estimate), ballistic conductance G through a CN should be unusual. Adopting the theory of Ref. 9 to the two-valley case, we find $G = e^2/h$, which is 1/4 of the non-interacting result, i.e., the "0.25-anomaly." On the other hand, G measured through a CN with resistive (tunneling) contacts may display an unusual power-law decrease[10] with T. The negative compressibility would reduce the charging energy of finite wires, and so Eq. (15) for $\varkappa$ can be tested by careful Coulomb blockade experiments on the CN quantum dots. Finally, the strong electron correlations can also be observed[25] in imaging microscopy: instead of the $4a$-periodic Friedel oscillations of a Fermi gas, charge density near boundaries of defects would oscillate with period a, i.e., four times smaller, in the CTG. With further descrease of n, these oscillations would become strongly anharmonic as appropriate for a pinned Wigner crystal. Detailed quantitative predictions for all such measurements will be discussed elsewhere.

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